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Examiner Marjorie Moran	US Patent and Trademark Office	703.746.5257	703.305.2363

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Kristin M. Joslyn	October 10, 2002	646.728.2893	212.596.9426

CLIENT	RE:	TIME	PAGES (INCLUDING COVER)
03666.031	United States Patent Application No. 09/431,469 <u>Our Ref.: VPI/95-09 DIV</u>		5

## MESSAGE

**Attn: EXAMINER MORAN**

Please forward the following draft proposed claim directly to Examiner Moran. The enclosed proposed claim is a draft document for discussion.

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October 10, 2002

**VIA FACSIMILE**

Examiner Marjorie Moran  
US Patent and Trademark Office

United States Patent Application No. 09/431,469  
Our Ref.: VPI/95-09 DIV

Dear Examiner Moran:

Thank you for your helpful discussions in the above-identified application.

I enclose a draft claim 19 for your review. Please contact me at your earliest convenience to discuss the proposed amendments. I also enclose an Associate Power of Attorney as you requested.

Thank you for your help.

Very truly yours,

Kristin M. Joslyn  
Patent Agent

KJ:kj  
Enclosures

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Application No. 09/431,469

VPI/95-09 DIV

**DRAFT**

19. A method of using a computer for evaluating the ability of a plurality of chemical [entity] entities to associate with a crystallized molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:
- a. positioning one of said plurality of chemical entities within the CnA binding pocket or the CnA homologue binding pocket;
  - b. employing computational means which utilize said structure coordinates to perform a fitting operation between [the] said chemical entity and the CnA binding pocket or the CnA homologue binding pocket;
  - [b]c. analyzing the results of said fitting operation to quantify the association between [the] said chemical entity and the CnA binding pocket or the CnA homologue binding pocket; [and]
  - [c]d. outputting said quantified association to a suitable output hardware;
  - e. optionally repeating steps a. through d. with another of said plurality of chemical entities; and
  - f. selecting at least one of said plurality of chemical entities that associates with the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

**DRAFT**